# US-UK COLLABORATION ON VIRTUAL PLANT SIMULATION Notes of Meeting at NETL, Morgantown,

At 9am, Friday 27 May 2005

#### **Present:**

Steve Zitney

Ben Keeping

Tony Oliver

Maxwell Osawe

NETL

PSE

K-S Tech

Fluent (US)

### 1. Introduction

The objectives of the meeting were:

- To review developments in the US and UK
- To review progress in the collaboration
- To consider future developments within the collaboration

## 2. Notes of 2nd Video Conference Meeting and Matters Arising

Action 1.3 – once the current US solicitation is over and the awards made in early 2005, then the subcontracts in the relevant work areas will be pulled into the collaboration. This was discussed further in the meeting, see below

Action 1.7 – Solids specification – CAPE-OPEN (C-O) solids specification is being handled by the Thermo SIG in CO-LaN. At the preceding US C-O seminar, SZ had outlined the industry's requirements for solids handling. CO-LaN then described the solids handling capability that is being developed as part of the Thermo 1.1 specification. AspenTech has developed a prototype implementation of the solids handling capability in Aspen Plus 12.1 and Aspen Plus 2004. This will provide Aspen Plus users with access to streams comprising one MIXED and one CISOLID substream via the CAPE-OPEN interfaces. There currently does not appear to be any support for coal analysis or particle size distribution information.

Action 2.2 - The year one report covers IT security when operating across the internet and ALSTOM will take the lead in producing this. Agreed to divide this task into two parts 1) IT Security and 2) Protection of Intellectual Property (IP). NETL will get their IT people to contribute/review as appropriate. This is to be incorporated into the Task Sheets

Action 3.1 Tony/Steve

Action 2.3 - The year 3 report will cover intellectual property protection and NETL will ask the organisations that have been successful in their solicitations to contribute. This is to be incorporated into the Task Sheets

Action 3.2 Tony/Steve

- Action 2.4 The year one deliverable on the status of C-O dynamics should be used to help lobby CO-LaN for the development of C-O dynamics. This is to be incorporated into the Task Sheets

  Action 3.3 Tony/Steve
- Action 2.5 Complete. The US DOE have set up a web site for the US-UK collaboration on fossil energy R&D (<a href="http://us-uk.fossil.energy.gov/">http://us-uk.fossil.energy.gov/</a>). It has been agreed to use a protected area of the site as a document library for the partners in our collaboration. Publishing to the web site will be via US DOE.
- Action 2.6 Complete. It was not possible to meet after the US-UK Joint Coordinating Committee Meeting on May 2 in Alexandria, VA. A progress report on US-UK Virtual Power Plant collaboration was given by TO.
- Action 2.7 Complete. Ben Keeping and Tony Oliver attended the 2<sup>nd</sup> Annual U.S. CAPE-OPEN Meeting in NETL, Morgantown, WV on May 25-26, 2005
- Action 2.8 Complete. Arrangements for SZ to visit the UK for a meeting on the collaboration were discussed at this meeting; see below.

## 3. Update on US APECS Project

The NETL Advanced Process Engineering Co-Simulator (APECS) project is focusing on simulating the FutureGen power and hydrogen production plant. One potential FutureGen simulation is using CFD models of an entrained-flow gasifier and gas turbine combustor. NETL is working on additional device-scale models including a 3D FLUENT CFD model of an industrial-scale, syngas-fuelled gas turbine combustor model, and FLUENT and MFIX Eulerian-Eulerian CFD models for a commercial-scale "transport" gasifier to be used in developing ROMs for use in FutureGen plant simulation – further details of the multiphase flow code MFIX are given in www.mfix.org.

In the area of advanced power plant simulation, three DOE Clean Coal R&D awards have been made as part of the APECS initiative:

1. **Fluent, Inc.** (**Lebanon, N.H.**) - Fluent and partners will develop an integrated simulation capability by linking a hierarchy of plant- and equipment-level models that will have varying levels of fidelity and computational speed suitable for either preliminary conceptual design or detailed final design. A main objective of the project is to complete the development of an integrated steady-state simulator that will include computationally efficient reduced order models (ROM) and a 3D virtual reality walkthrough capability. A second objective is to develop a prototype dynamic simulator that integrates plant- and equipment-level models. The use of leading commercial, advanced capability software tools as the backbone of the simulator infrastructure will ensure that the infrastructure will remain supported and available to the industry far into the future for simulating advanced power plants. Team members include

ALSTOM Power, Inc., Windsor, Conn.; Aspen Technology, Inc., Cambridge, Mass.; and Carnegie Mellon University, Pittsburgh, Pa.. (DOE share: \$1,883,320; Project duration: 36 months)

- 2. Reaction Engineering International (Salt Lake City, Utah) Reaction Engineering International (REI) proposes to develop a virtual engineering based software framework to support static and dynamic plant engineering simulations, which will be used to assess and evaluate the performance of advanced power generation systems. A software system that supports virtual engineering functionality will be used to create the framework, and financial models will be used to implement plant economics. The VE Suite Virtual Engineering Framework (VEF) will include a hierarchy of models and visualization tools to construct, perform and interrogate simulation results for component models and overall plant performance at multiple levels of detail within a three-dimensional (3-D), user-centered, interactive environment. The VEF will enable researchers to better understand the interactions of different equipment components, identify weaknesses and processes needing improvement and thereby allowing more efficient, less expensive plants to be developed and brought on line faster and in a more cost-effective manner. Team members include American Electric Power (AEP), Columbus, Ohio; AmerenUE, St. Louis, Mo.; Praxair, Tonawanda, N.Y.; MIT, Belmont, Mass.; EPRI, Palo Alto, Calif.; Iowa State University, Ames, Iowa; Carnegie Mellon University, Pittsburgh, Penn.; Cooperative Research Centre For Coal in Sustainable Development, Newcastle, Australia; and Enertechnix, Maple Valley, Wash.. (DOE share: \$440,998; Project duration: 24 months)
- 3. Texas A&M University (College Station, Texas) A method will be developed that will drastically reduce the computational effort required to model multiphase flow reactors such as circulating fluidized-bed combustors and fluid catalytic cracking risers. This reduction will be accomplished by developing a low order model based on the proper orthogonal decomposition (POD) method. In this project, a reduced order model for multiphase flow reactors previously developed by the investigator will be enhanced to better capture the flow physics, to reduce the computational time and to provide interfaces that allow for integration with power plant simulations. The development of the reduced order model will significantly impact the design of new reactors by improving the understanding of multiphase flow and chemical reactions. (DOE share: \$298,974; Project duration: 36 months)

Steve is to consider how best to bring these awarded projects into the virtual plant simulation collaboration

Action 3.4 Steve

NETL are planning to build up their dynamics modelling capability in Steve's group and the plan is to include the development of an IGCC training simulator.

## 4. Update on UK's VPDM Project

The first draft of the Functional Specification is now complete and the preliminary design of the architecture is now finalised. The architecture has a FIPER ACS on the PME site communicating across the intent to a FIPER ACS on the PMC site. The first IT installation at a partner's site is also nearing completion and preliminary testing is being carried out on security and communication through the partner's firewalls.

A prototype stand-alone CAPE-OPEN (C-O) socket, which is one of the key components, is now complete and has been successfully tested with a simple legacy code belonging to one of the partners, which has been wrapped. Development of the other software components of the architecture is continuing and the C-O socket for gPROMS should be completed soon.

Work has now started on the wrapping of the proprietary, legacy codes for a furnace, boiler and three steam turbine stages. The chosen variants of these models all correspond to an existing pulverised coal power station and one of the key tests for the VPDM will be to model this power station using these proprietary models which will reside on their owners IT system. Each of these models has their own integrated calculations for physical properties and a means of ensuring consistency in properties is being looked at.

Preliminary discussions have started on implementing FLUENT with the V21 Controller. Some development work is likely to be needed, as anticipated in the project.

Two approaches for Reduced Order Models (ROM) for use with the VPDM are to be investigated – a zone model approach and a neural network approach. Work on the neural net approach has started but work on the zone model approach is scheduled for later in the project.

An additional activity in the project is the development and implementation of the University of Ulster code ECLIPSE in the VPDM. This is a PME developed for power plant modelling and it is not C-O compliant. Work has started on making ECLIPSE C-O compliant with a C-O socket for plugging in C-O PMCs.

The first major test of the VPDM will be its application to a pulverised coal station using distributed non-proprietary, simple PMCs; these are likely to be models for the furnace, boiler and steam turbines. This will be followed by test with the non-proprietary models replaced by the proprietary ones for the same application. The final test of the VPDM will be for a new technology with carbon capture with the technology being chosen by the partners in collaboration with the DTI.

#### 5. Collaboration Tasks

Collaboration on all four tasks is continuing through the meetings. The first deliverables, which are reports on reduced-order modelling and internet security for proprietary

models, are due at the end of 2005. A meeting in the UK on the collaboration is being scheduled for autumn 2005 (see below) and this will be used to initiate the production of the joint reports.

## 6. Next Meeting

The next meeting is to be held in UK in autumn 2005. This will include a collaboration progress meeting, probably in London, together with visits to PSE in London and to Fluent (Europe) in Sheffield; this is to be arranged

Action 3.5 Tony/Steve

Tony Oliver, Steve Zitney, June 2005